LCF: Ab-initio Nuclear Structure Computations

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“Given a lump of nuclear material, what are its properties, and how does it interact?”

How are we going to describe nuclei that we cannot measure?

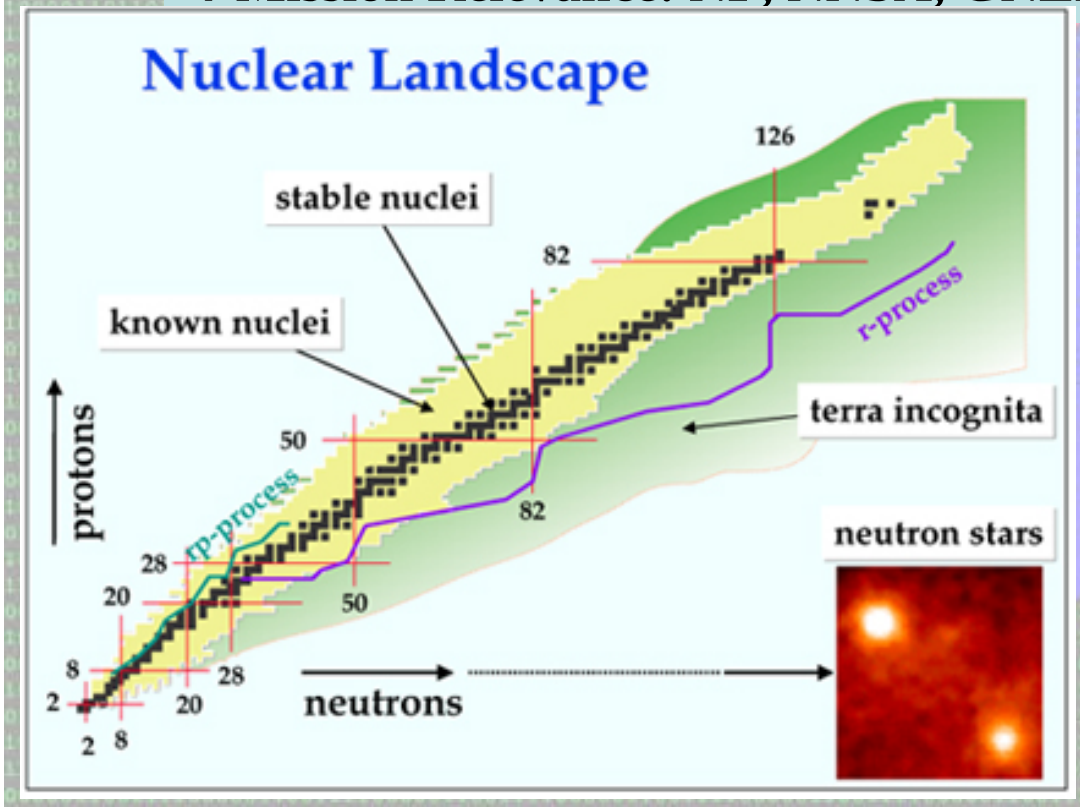
→Robust and predictive nuclear theory for structure and reactions

→Need for nuclear data to constrain theory

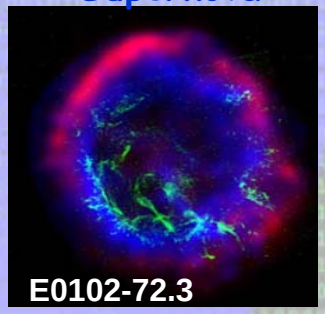
→We are after the Hamiltonian

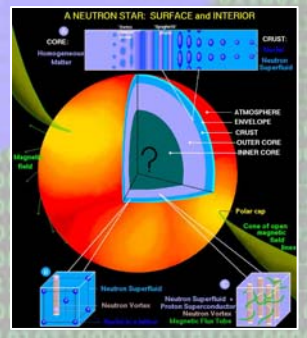
- **→bare intra-nucleon Hamiltonian**
- **→energy density functional**

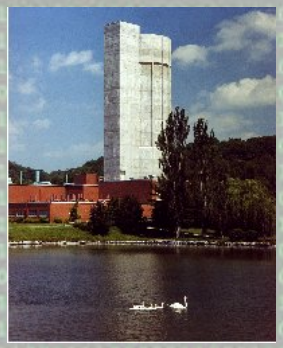
→Mission Relevance: NP, NNSA, GNEP



Supernova







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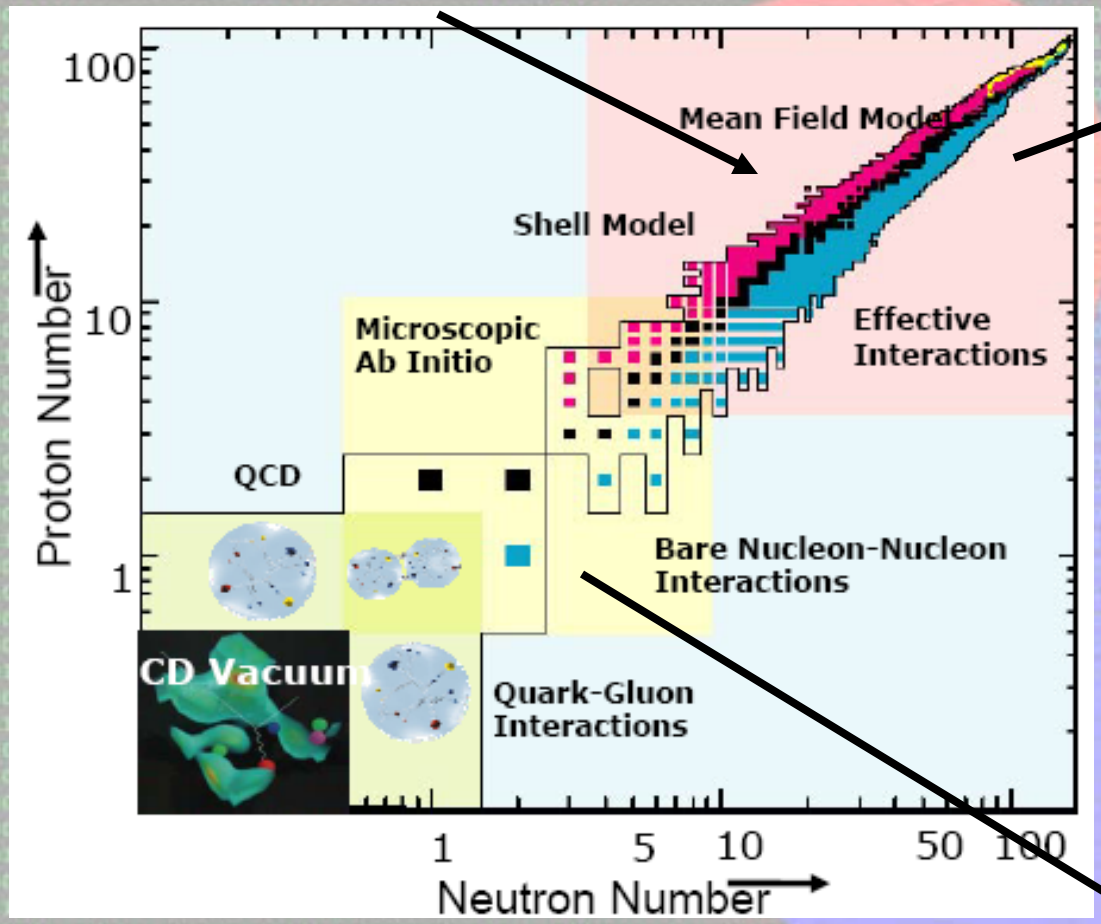
Pushing the nuclear boundaries

Thermal Properties region

Nuclear DFT effort



The LCF effort will:

- **Enlarge the ab-initio square**
- **Enable initial global DFT calculations with restored symmetries.**
- **Explore thermal nuclear properties in the mass 80-150 region.**

ALL REGIONS: Nuclear cross section efforts (NNSA, RIA, Nuclear Energy)

Nuclear Coupled Cluster effort

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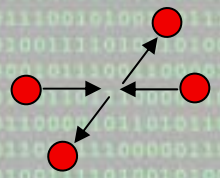
Nuclear interactions



Nasty, spin and isospin dependent 2-body forces

$$H = \sum_{i=1,A} \frac{-\hbar^2}{2M_i} \nabla_i^2 + \sum_{i<j} V(r_i, r_j) + V_{NNN}$$

Real three-body interactions

Solved up to mass 12 with GFMC, converged mass 8 with diagonalization. We want to go much further!

$$H|\Psi\rangle = E|\Psi\rangle$$

Nuclear Coupled-Cluster Theory

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Coupled Cluster Theory: ab initio in medium mass nuclei

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$

Correlated Ground-State wave function — **Correlation operator** — **Reference Slater determinant**

$$T = T_1 + T_2 + T_3 + \cdots$$

$$T_1 = \sum_{\substack{i<\varepsilon_f \\ a>\varepsilon_f}} t_{ai} a_a^+ a_i$$

$$T_2 = \sum_{\substack{ij<\varepsilon_f \\ ab>\varepsilon_f}} t_{abij} a_a^+ a_b^+ a_j a_i$$

Energy

$$E = \langle \Phi | \exp(-T) H \exp(T) | \Phi \rangle$$

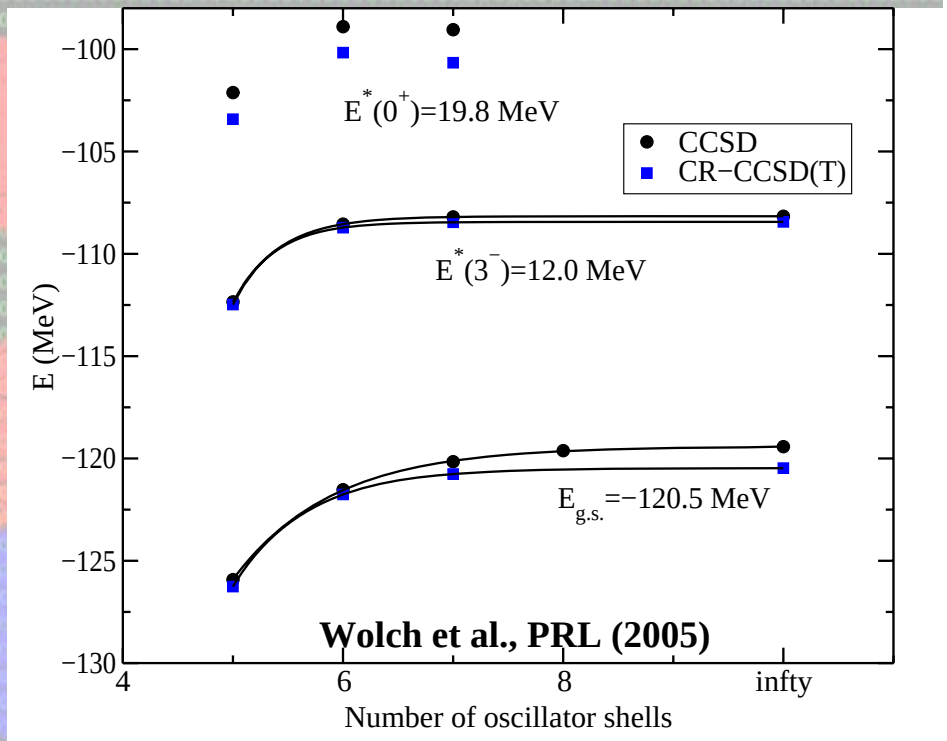
Amplitude equations

$$\langle \Phi_{ij\cdots}^{ab\cdots} | \exp(-T) H \exp(T) | \Phi \rangle = \langle \Phi_{ij\cdots}^{ab\cdots} | \overline{H} | \Phi \rangle = 0$$

- Boils down to a set of coupled, nonlinear algebraic equations
- Storage of both amplitudes and interactions is an issue as we scale up.
- Largest problem so far: 40Ca with 2 million unknowns, 7 peta-ops to solve once (up to 10 runs per publishable result)
- Breakthrough science: inclusion of 3-body force into CC formalism (6d tensor)

Coupled cluster theory: ab initio in heavier nuclei

The effect of 3-body clusters on states.
- **Collaborations with P. Piecuch (MSU)**
- **Implemented CR-CCSD(T) for the nuclear problem.**
- **Calculated excited states with EOMCCSD and CR-EOMCCSD(T)**
- **Calculated A+/-1 systems.**



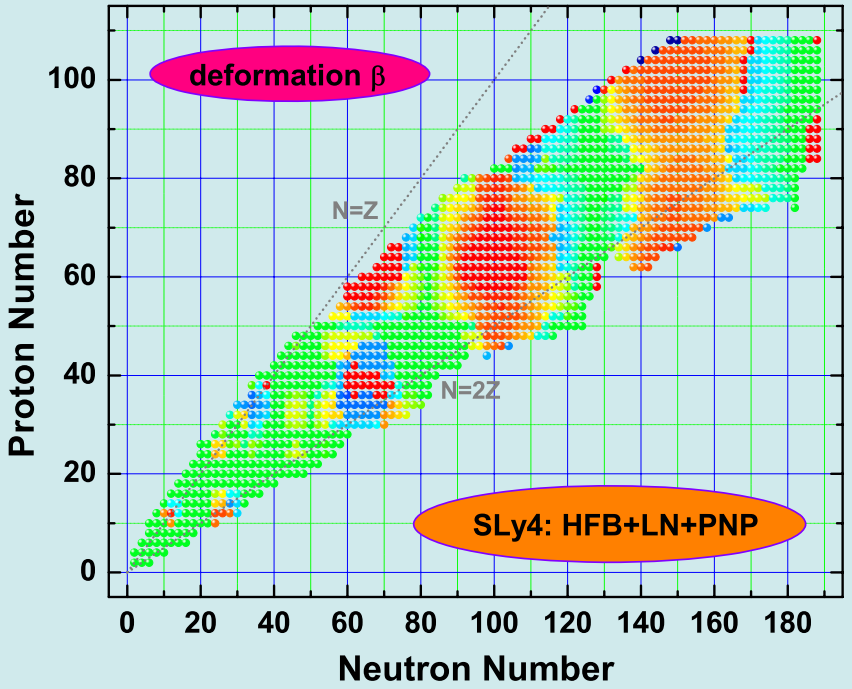
RESULTS:
- **Excited state is high with the two-body force alone (lack of good 'l-splitting').**
- **Triples amplitudes are small and have little effect on states**
- **Different forces yield different spin-orbit splittings.**
- **Some further oscillater dependence in A+/-1 systems than in A.**

Dean & Hjorth-Jensen, PRC69, 054320 (2004); Kowalski, Dean, Hjorth-Jensen,Papenbrock, Piecuch, PRL92, 132501 (2004); Wloch, Dean, Gour, Hjorth-Jensen, Papenbrock, Piecuch, PRL94, 21501 (2005); Gour, Piecuch, Wloc, Hjorth-Jensen, Dean submitted to PRC (2005).

Self-consistent mean field theory: Nuclear DFT

Major Involvement:
Nazarewicz, Stoitsov, Skalski, Borycki, Nikolov

Stoitsov, et al., Phys. Rev. C68, 054312(2003)



Basic Points:

- General nuclear energy density functional that allows proton-neutron couplings
- First fully self-consistent QRPA+HFB
- Development of formalism for exact particle number projection before variation
- Mass tables produced in parallel.

Future plans:

- Implement exact particle number projection before variation
- Improvement of the density dependence of the effective interaction
- Proper treatment of time-odd fields
- Inclusion of dynamical zero-point fluctuations
- Provide proper continuum basis for QRPA calculations

Stoitsov, Dobaczewski, Nazarewicz, Pittel, Dean, PRC68, 054312 (2003); Terasaki, Engel, Bender, Dobaczewski, Nazarewicz, Stoitsov, PRC71, 34310 (2005); Cwiok, Heenen, Nazarewicz, Nature 433, 705 (2005)